Low Mach number modeling of type Ia supernovae

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Applied Mathematics Seminar
UC Berkeley
October 1, 2007

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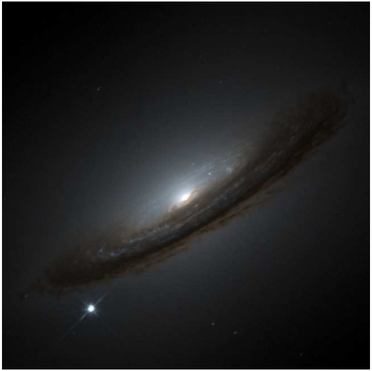
Type Ia Supernovae (SNe Ia)

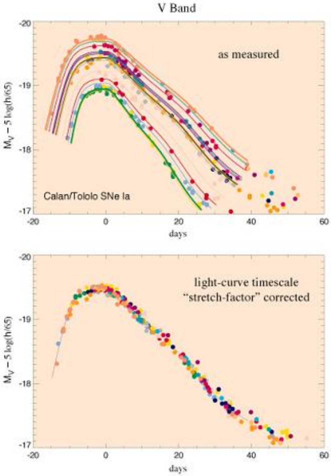
Type Ia supernovae



- Brightness rivals that of host galaxy, L $\approx 10^{43}$ erg / s
- Definition: no H line in the spectrum, Si II line at 6150A.
- Mechanism: thermonuclear explosion of white dwarf

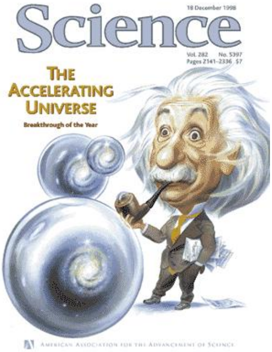
Light Curves

- Key observable for SNe Ia is the light curve (brightness vs time).
- Light curves from different SNe Ia have similar shape, except for brighter $\approx$ broader.
- With a single “time stretch” factor we can map all these curves onto a single curve.



1998 Science Breakthrough of the Year

(Supernova Cosmology Project and High-z Supernova Search Team)



- By observing the duration of distant SNe Ia one could determine their absolute magnitude (standard candles).
- absolute vs. apparent brightness $\rightarrow$ distance
- distance vs. redshift $\rightarrow$ Hubble diagram.

This led to the discovery that the rate at which the Universe is expanding is increasing.

Type Ia Supernovae Theory

- The best model for SNe Ia is the thermonuclear explosion of a carbon/oxygen white dwarf. This is a very compact star, about the size of the Earth but more massive than the Sun ($\approx$ 5-10 billion years to become a white dwarf).
- In a white dwarf, electrons provide the needed pressure (electron degeneracy); unlike an ideal gas, an electron gas exhibits a pressure even at zero temperature.
- Chandrasekhar showed that the maximum mass that can be supported by electron degeneracy pressure is 1.4 times the mass of the sun.
- If the white dwarf is in a close binary orbit with a large companion star that is still actively burning, there can be a steady stream of material from the active star slowly accreting onto the white dwarf ($\approx$ 10 million years to reach the Chandrasekhar limit).

Then...

Type Ia Supernovae Theory (p2)

- As the mass $\uparrow$, pressure $\uparrow$ and temperature $\uparrow$ and thermonuclear burning begins - carbon nuclei begin to fuse.
- Heating $\rightarrow$ convection: plumes rise upward and cool via expansion ($\approx$ 100 years of convection)
- Eventually, cooling through convection can no longer balance the heat generation through reactions. Simmering becomes ignition.
- Initially at least, the flame front is a deflagration (subsonic), allowing the star to expand. The flame front accelerates, possibly becoming a detonation.
- Finally, the star explodes ($\approx$ 1 second from ignition to explosion).

The fact that all SNe Ia begin with approximately the same mass explains their similarities. The differences in carbon/oxygen ratios, and accretion and rotation rates, may explain the differences.

Modeling of Type Ia Supernovae

Typically, numerical simulations of SNe Ia have used the compressible Navier-Stokes equations with reactions:

$$
\begin{aligned}
\rho_t + \nabla \cdot \rho U &= 0 \\
(\rho U)_t + \nabla \cdot (\rho U U + p) &= -\rho g \mathbf{e}_r \\
(\rho E)_t + \nabla \cdot (\rho U E + U p) &= \nabla \cdot \kappa \nabla T - \rho g (U \cdot \mathbf{e}_r) + \rho H \\
(\rho X_m)_t + \nabla \cdot \rho U X_m &= \rho \dot{\omega}_m
\end{aligned}
$$

ρ	density	e	internal energy
U	flow velocity	X_m	mass fractions
p	pressure	$\dot{\omega}_m$	production rate
T	temperature	$\vec{g}$	force of gravity
$E = e + U^2/2$	total energy	$H = \sum_m \rho q_m \dot{\omega}_m$	heating

Modeling cont'd

Timmes equation of state provides:

$$e(\rho, T, X_k) = e_{ele} + e_{rad} + e_{ion} \qquad p(\rho, T, X_k) = p_{ele} + p_{rad} + p_{ion}$$

$$\begin{aligned} e_{ele} &= \text{fermi} \\ e_{rad} &= aT^4/\rho \\ e_{ion} &= \frac{3kT}{2m_p} \sum_m X_k/A_m \end{aligned} \qquad \begin{aligned} p_{ele} &= \text{fermi} \\ p_{rad} &= aT^4/3 \\ p_{ion} &= \frac{\rho kT}{m_p} \sum_m X_k/A_m \end{aligned}$$

Standard approach: explicit integration of compressible equations with AMR

- Hillebrandt, Niemeyer et al. at MPI, Garching
- Oran et al. at NRL
- Rossner, Kokhlov, Plewa, et al. at U. Chicago

However, early phases of the problem are characterized by low Mach number flows

- Convection leading up to ignition
- Flame propagation

Simulation strategy

A numerical simulation using an explicit method based on the compressible formulation, such as FLASH, would use a time step based on the sound speed.

- require too many time steps for long-time integration,
- be badly conditioned for low-speed flows ($\pi/p_0 = O(M^2)$)

Develop low Mach number methodology to simulate Type Ia, at least up until near the final phase of the explosion

- Generalize low Mach number formulation to general equation of state
  - Eliminate acoustic time-step restriction while retaining compressibility effects due to heat release and stratification
  - Conserve species and enthalpy
- Projection formulation
- Adaptive mesh refinement

Low Mach Number Approach

Asymptotic expansion in the Mach number, $M = |U|/c$, leads to a decomposition of the pressure into thermodynamic and dynamic components:

$$p(\mathbf{x}, t) = p_0(r, t) + \pi(\mathbf{x}, t)$$

where $\pi / p_0 = O(M^2)$.

- p_0 affects only the thermodynamics; π affects only the local dynamics,
- Physically: acoustic equilibration happens infinitely fast; sound waves are “filtered” out
- Mathematically: resulting equation set is no longer strictly hyperbolic; a constraint equation is added to the evolution equations
- Computationally: time step is dictated by fluid velocity, not sound speed.

Low Mach Number Nuclear Flames

Generalize low Mach number combustion to stellar EOS – small scales

$$
\begin{aligned}
&\rho_t + \nabla \cdot \rho u = 0 \\
&(\rho X_m)_t + \nabla \cdot \rho u X_m = \rho \dot{\omega}_m \\
&(\rho u)_t + \nabla \cdot (\rho u u) + \nabla \pi = \rho \vec{g} \\
&(\rho h)_t + \nabla \cdot (\rho u h) = \nabla \cdot \kappa \nabla T
\end{aligned}
$$

ρ	density		
X_m	mass fractions	T	temperature
$\dot{\omega}_m$	production rate	$\vec{g}$	force of gravity
u	flow velocity	π	perturbational pressure
$h = e + p/\rho$	enthalpy		

Together with a constraint equation $p(\rho, T, X_m) = p_{\text{amb}}$

How do we solve this constrained system of PDE's.

$\nabla \cdot U$ Constraint

For small-scale systems p_0 is constant along particle paths.

Differentiate constraint along particle paths

$$\nabla \cdot U = \frac{1}{\rho \frac{\partial p}{\partial \rho}} \left(\frac{1}{\rho c_p} \frac{\partial p}{\partial T} \left(\nabla \cdot \kappa \nabla T - \rho \frac{\partial h}{\partial X_m} \dot{\omega}_m \right) + \frac{\partial p}{\partial X_m} \dot{\omega}_m \right) \equiv S$$

How do we integrate this system?

Incompressible Navier Stokes Equations

Incompressible Navier Stokes equations provides a prototype for these types of constrained systems

$$U_t + U \cdot \nabla U + \nabla \pi = \mu \Delta U$$

$$\nabla \cdot U = 0$$

How do we develop efficient integration schemes for this type of system?

Vector field decomposition

$$V = U_d + \nabla \phi$$

where $\nabla \cdot U_d = 0$

and

$$\int U \cdot \nabla \phi dx = 0$$

We can define a projection **P**

$$\mathbf{P} = I - \nabla(\Delta^{-1})\nabla \cdot$$

such that $U_d = \mathbf{P}V$

Solve

$$-\Delta \phi = \nabla \cdot V$$

Projection method

Incompressible Navier Stokes equations

$$U_t + U \cdot \nabla U + \nabla \pi = \mu \Delta U$$

$$\nabla \cdot U = 0$$

Projection method

Advection step

$$\frac{U^* - U^n}{\Delta t} + U \cdot \nabla U = {}^1\!/\!_2 \mu \Delta (U^* + U_n) - \nabla \pi^{n-1/2}$$

Projection step

$$U^{n+1} = \mathbf{P} U^*$$

Recasts system as initial value problem

$$U_t + \mathbf{P}(U \cdot \nabla U - \mu \Delta U) = 0$$

LMN approaches

Can this approach be generalized to low Mach number flows?

- Finite amplitude density variations
- Compressiblility effects

Constant coefficient "projection"

- McMurtry, Riley, Metcalfe, AIAA J., 1986.
- Rutland & Fertziger, C&F, 1991.
- Zhang and Rutland, C&F, 1995.
- Cook and Riley, JCP, 1996.
- Najm, Trans. Phen. in Comb., 1996
- Najm & Wyckoff, C&F, 1997.
- Quian, Tryggvason & Law, JCP 1998.
- Najm, Knio & Wyckoff, JCP, 1998.

Variable coefficient projection

- Bell & Marcus, JCP, 1992.
- Lai, Bell, Colella, 11th AIAA CFD, 1993.
- Pember et al., Comb. Inst. WSS, 1995.
- Tomboulides et al., J. Sci. Comp., 1997.
- Pember et al., CST, 1998.
- Schneider et al., JCP, 1999.
- Day & Bell, CTM, 2000.
- Nicoud, JCP, 2000.

Variable coefficient projection

Generalized vector field decomposition

$$V = U_d + \frac{1}{\rho}\nabla\phi$$

where $\nabla \cdot U_d = 0$ and $U_d \cdot n = 0$ on the boundary

Then U_d and $\frac{1}{\rho}\nabla\phi$ are orthogonal in a density weighted space.

$$\int \frac{1}{\rho}\nabla\phi \cdot U \; \rho \, dx = 0$$

Defines a projection $\mathbf{P}_\rho = I - \frac{1}{\rho}\nabla((\nabla \cdot \frac{1}{\rho}\nabla)^{-1})\nabla\cdot$ such that $\mathbf{P}_\rho V = U_d$.

$\mathbf{P}_\rho$ is idempotent and $||\mathbf{P}_\rho|| = 1$

Generalized vector field decomposition

Use variable-ρ projection to define a generalized vector field decomposition

$$V = U_d + \nabla\xi + \frac{1}{\rho}\nabla\phi$$

where

$$\nabla \cdot \nabla\xi = S$$

and

$$\nabla \cdot U_d = 0$$

We can then define

$$U = \mathbf{P}_\rho(V - \nabla\xi) + \nabla\xi$$

so that $\nabla \cdot U = S$ with $\mathbf{P}_\rho(\frac{1}{\rho}\nabla\phi) = 0$

- This construct allows us to define a projection algorithm for variable density flows with inhomogeneous constraints
- Requires solution of a variable coefficient elliptic PDE
- Allows us to write system as a pure initial value problem

Low Mach number algorithm

Numerical approach based on generalized projection

Fractional step scheme

- Advance velocity and thermodynamic variables
  - Advection
  - Diffusion
  - Stiff reactions
- Project solution back onto constraint

Stiff kinetics relative to fluid dynamical time scales

$$\frac{\partial(\rho X_m)}{\partial t} + \nabla \cdot (\rho U X_m) = \rho \dot{\omega}_m$$

$$\frac{\partial(\rho h)}{\partial t} + \nabla \cdot (\rho U h) = \nabla \cdot (\lambda \nabla T)$$

Operator split approach

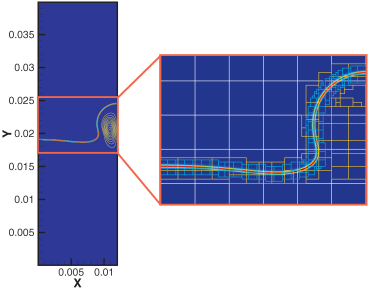
- Reactions $\Rightarrow \Delta t/2$
- Advection – Diffusion $\Rightarrow \Delta t$
- Reactions $\Rightarrow \Delta t/2$

AMR – exploit varying resolution requirements in space and time
Block-structured hierarchical grids

- Amortize irregular work

Each grid patch (2D or 3D)

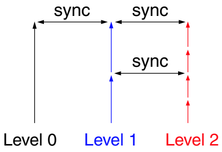
- Logically structured, rectangular
- Refined in space and time by evenly dividing coarse grid cells
- Dynamically created/destroyed



2D adaptive grid hierarchy

Subcycling:

- Advance level ℓ, then
  - Advance level $\ell + 1$
    level ℓ supplies boundary data
  - Synchronize levels ℓ and $\ell + 1$



AMR Synchronization

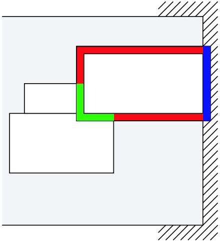
Coarse grid supplies Dirichlet data as boundary conditions for the fine grids.

Errors take the form of flux mismatches at the coarse/fine interface.

Design Principles:

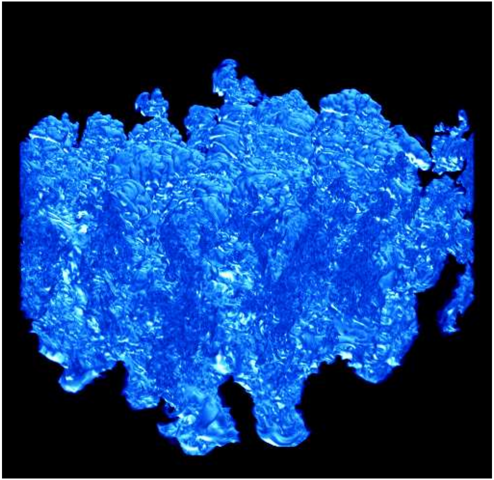
- Define what is meant by the solution on the grid hierarchy.
- Identify the errors that result from solving the equations on each level of the hierarchy “independently”.
- Solve correction equation(s) to “fix” the solution.
- Correction equations match the structure of the process they are correcting.

- Fine-Fine
- Physical BC
- Coarse-Fine

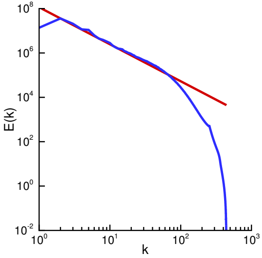


Preserves properties of single-grid algorithm

3D Rayleigh Taylor Flame



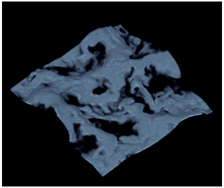
Flame surface

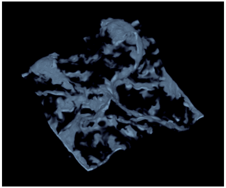


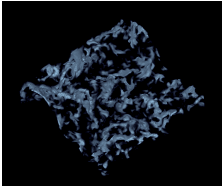
Turbulent energy spectrum

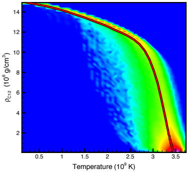
Turbulence / Flame interactions

As flame propagates outward it becomes thicker and slower

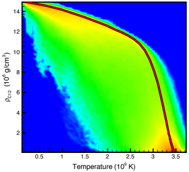




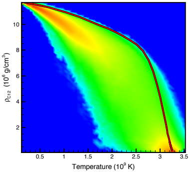




$\rho = 4.0 \times 10^7$



$\rho = 3.0 \times 10^7$



$\rho = 2.35 \times 10^7$

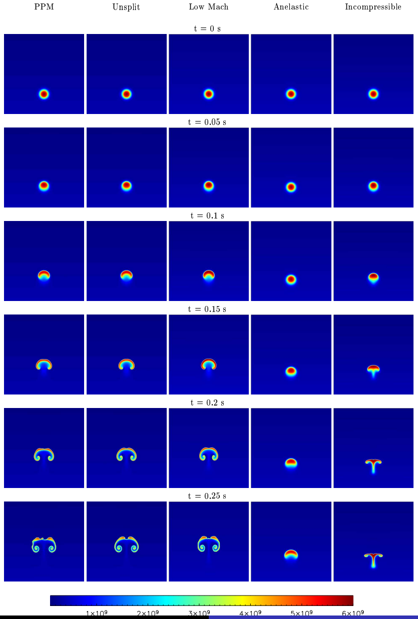
Larger scale models

For larger scales we need to include effects of background stratification

Possible models for convective motion:

- Boussinesq: next simplest model - allows heating-induced buoyancy in a constant density background (constant p_0, ρ_0, T_0)
- Variable-ρ incompressible: finite amplitude density variation but incompressible
- anelastic: allows small variations in temperature and density from a stratified background state ($p_0(r), \rho_0(r), T_0(r)$)
- low Mach number : large variations in temperature and density in a time-varying stratified background state ($p_0(r,t), \rho_0(r,t), T_0(r,t)$)

Special case: Small-Scale Heating



Low Mach Number Model

$$\begin{aligned}
\frac{\partial(\rho X_k)}{\partial t} &= -\nabla \cdot (U \rho X_k) + \rho \dot{\omega}_k \quad , \\
\frac{\partial(\rho h)}{\partial t} &= -\nabla \cdot (U \rho h) + \frac{D p_0}{D t} - \sum_k \rho q_k \dot{\omega}_k + \rho H_{\mathrm{ext}} \quad , \\
\frac{\partial U}{\partial t} &= -U \cdot \nabla U - \frac{1}{\rho} \nabla \pi - \frac{(\rho - \rho_0)}{\rho} g \mathbf{e}_r \quad , \\
\nabla \cdot (\beta_0 U) &= \beta_0 \left(S - \frac{1}{\Gamma_{10} p_0} \frac{\partial p_0}{\partial t} \right) \quad ,
\end{aligned}$$

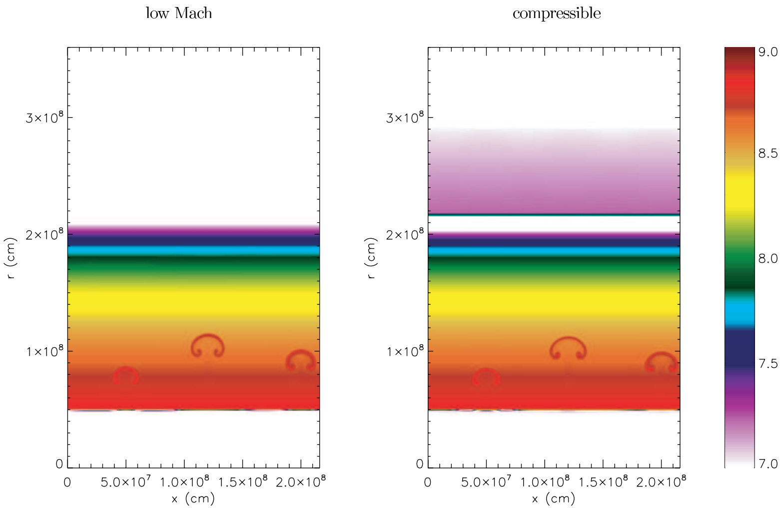
Cannot assume fixed background for net large-scale heating We need evolution equations for p_0, ρ_0, etc.

Use average heating to evolve base state. Remaining dynamics evolves perturbations

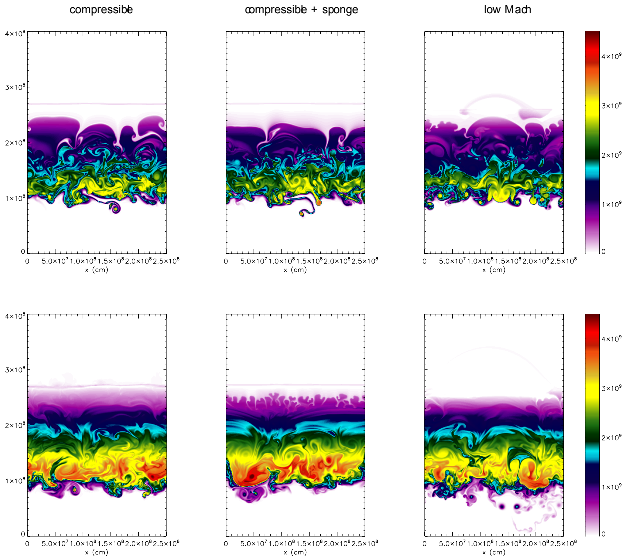
$$\frac{\partial p_0}{\partial t} = -w_0 \frac{\partial p_0}{\partial r} \quad \text{where} \quad \mathrm{w}_0(\mathrm{r}, \mathrm{t}) = \int_{\mathrm{r}_0}^{\mathrm{r}} \overline{\mathrm{S}}(\mathrm{r}', \mathrm{t})\, \mathrm{dr}'$$

Self gravity introduces additional complexity

Compressible Comparison

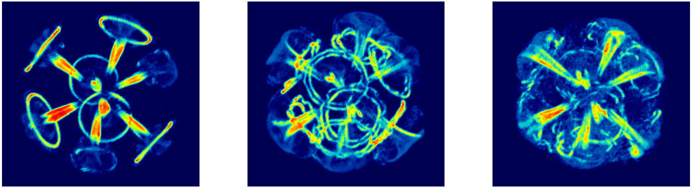


Compressible Comparison



3D simulation of stellar convection

Vorticity



- Simulation of spherical star in 3D Cartesian grid
- Initial with one-dimension white dwarf model
- Motion driven by specified heat source
- Simulation on 256^3 domain
- Radial sponge to damp spurious motion at edge of star

Summary

We have developed a new methodology for modeling Type Ia supernovae, based on low Mach number asymptotics that allows us to filter acoustic waves without making overly restrictive assumptions about the variation from the base state.

- Allow background state to evolve in both space and time.
- Projection methodology for solving the new system is well-established and well-tested for many other applications; extends naturally to SNe Ia.
- Results using the low Mach number approach show excellent agreement in the range where both approaches are valid.
- Low Mach number model shows large efficiency gains over compressible codes for evolving low-speed flows.
- Currently extending this model to full-star modeling.
- Physics investigations
  - Study conditions leading up to SN Ia ignition
  - Model deflagration stage of SN Ia – requires flame model
  - X-ray bursts, Nova